

# Boundary interactions changing operators and dynamical correlations in quantum impurity problems.

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Recent developments have made possible the computation of equilibrium dynamical correlators in quantum impurity problems. In many situations however, one is rather interested in correlators subject to a non equilibrium initial preparation; this is the case for instance for the occupation probability  $P(t)$  in the double well problem of dissipative quantum mechanics (DQM). We show in this paper how to handle this situation in the framework of integrable quantum field theories by introducing “boundary interactions changing operators”. We determine the properties of these operators by using an axiomatic approach similar in spirit to what is done for form-factors. This allows us to obtain new exact results for  $P(t)$ ; for instance, we find that at large times (or small  $g$ ), the leading behaviour for  $g < \frac{1}{2}$  is  $P(t) \propto e^{-\Gamma t} \cos \Omega t$ , with the universal ratio.  $\frac{\Omega}{\Gamma} = \cot \frac{\pi g}{2(1-g)}$ .

Strongly correlated electron systems, which have been the subject of intense study in recent years, pose many theoretical challenges due to their essentially non perturbative nature. The greatest progress have been realized for systems that are one dimensional, in particular quantum impurity problems. Fixed points and their vicinity can then be investigated with techniques of conformal field theory (CFT) [1], and the behaviour between fixed points with the Bethe ansatz [2], [3]. Even with these powerful tools, the understanding of dynamical properties is still quite incomplete. For instance the Bethe ansatz provides thermodynamic properties, and, with some effort, DC properties, including out of equilibrium [4]; but time and space dependent correlations, though accessible in principle [5], have remained largely undetermined until recently. It is highly desirable to make progress in that area, in particular in view of recent exciting experiments [6], [7].

In the last two years, building on formal works on integrable massive quantum field theories (QFTs) [9], [10], [11], it has become possible to determine some of these correlators exactly (ie with arbitrary accuracy, all the way from short to large distances) [12]. The results obtained sometimes exhibit striking behaviour, illustrating the difficulty to build an intuition for non perturbative systems. For instance, in the double well problem of dissipative quantum mechanics, it was found that the transition from coherent to incoherent regime, if based on the two spin correlation function, takes place at a value of the dissipation  $\alpha = \frac{1}{3}$  [12], [13], in contrast with the value  $\alpha = \frac{1}{2}$  expected before [14], [15]. This result later raised questions about which quantity should be used to describe this transition [16].

Unfortunately, correlators that can be computed in the framework of QFT are not always the physically relevant ones. This is because natural objects in QFT are vacuum vacuum Green functions, while in many experimental settings, what is measurable are time evolutions for a system prepared in a given state that is, in fact, not even an eigenstate. A well known example of this is the occupation probability  $P(t)$  in the double well problem of DQM [14]. In that problem, the system has a non equilibrium initial preparation: for negative times, the spin is held fixed in the state  $S_z = 1$ , with an equilibrated environment. At time  $t = 0$ , the constraint is released, and the dynamics starts from  $P(0) = 1$  with a factorized spin-environment initial state. The behaviour of  $P(t)$  has been the subject of much work lately [17], [18]. Several possibilities for measuring this quantity experimentally have also been proposed [19], [20]. On the other hand, no exact result for  $P(t)$  has been available up to now, except at  $\alpha = \frac{1}{2}$  [14].

In this letter, we introduce a method to compute correlators in prepared initial states that are not eigenstates. The key ingredient is a generalization of the boundary conditions changing operators of CFTs [1], [21] to theories with boundary interactions. We illustrate the method by the computation of  $P(t)$ . The final results are too bulky to be presented here; they have the following interesting features. For  $g > \frac{1}{2}$ , the behaviour of  $P(t)$  is incoherent, and  $P(t)$  has the general form

$$P(t) = \sum_{n=1}^{\infty} a_n e^{-2nT_b t} \quad (1)$$

where  $\sum a_n = 1$ , and  $T_b$  is an energy scale characterizing the tunnel splitting of the free system (see below). The transition from coherent to incoherent regime takes place at  $g = \frac{1}{2}$ , and is related with the transition from repulsive to attractive regime in the sine-Gordon model. For  $g < \frac{1}{2}$ ,  $P(t)$  has a form similar to (1) but the sum involves also (known) complex arguments in the exponential. At large times, the dominant behaviour is

$$P(t) \simeq \exp \left[ -2tT_b \sin^2 \frac{\pi g}{2(1-g)} \right] \cos \left[ tT_b \sin \frac{\pi g}{1-g} \right] \quad (2)$$

which in turn leads to the prediction for the ratio of the damping factor to the period of oscillations

$$\frac{\Omega}{\Gamma} = \cot \frac{\pi g}{2(1-g)}. \quad (3)$$

All these results are new, except for the fact that the transition occurs right at  $g = \frac{1}{2}$ , which was demonstrated using perturbation around  $g = \frac{1}{2}$  in [17].

To start, we recall the concept of boundary conditions changing operator, and we introduce their generalization, in the simple case of the Ising model (closely related to the double well problem at  $g = \frac{1}{2}$ ). We consider the massive Ising model with an inhomogeneous boundary magnetic field

$$A = \int_{-\infty}^0 dx \int_{-\infty}^{\infty} dy a_{FF}(x, y) \quad (4)$$

$$+ \frac{1}{2} \int_{-\infty}^{\infty} dy [(\psi\bar{\psi})(x=0) + a\bar{a}] + \int_{-\infty}^{\infty} dy h(y) \sigma_B(y),$$

where  $a_{FF}$  is the usual massive free Majorana fermion action,  $a$  is a boundary fermion satisfying  $a^2 = 1$ ,  $\sigma_B$  is the boundary spin operator, which coincides with  $\frac{1}{2}(\psi + \bar{\psi})a$ . If the mass vanishes, the theory is conformal invariant in the bulk. Conformal invariant boundary conditions are then obtained with  $h = 0$  (free spins) or  $h = \pm\infty$  (fixed spins). As shown by Cardy [21], the situation where boundary conditions are conformal invariant but inhomogeneous can be represented by the insertion of conformal operators on the boundary. For instance, the case with  $h = 0$  for  $y \leq 0$  and  $h = \infty$  for  $y > 0$  is described by the insertion of the operator  $\Phi_{12}$  of dimension  $\Delta = \frac{1}{16}$  at  $y = 0$ .

Let us now consider a situation where conformal invariance is broken: first suppose that the bulk mass is non zero, and that the boundary magnetic field is uniform and equal to  $h_a$ . This can be handled using the integrability of the problem [8], [9]. The hamiltonian (for time evolution along the  $y$  direction) is diagonalized using a basis of multiparticle states (here, simply fermions) that have factorized scattering both in the bulk and at the boundary. We use in the following rapidity variables parametrizing energy and momentum as  $e = m \cosh \theta$ ,  $p = m \sinh \theta$ ; the asymptotic states have then the general form  $|\theta_1, \dots, \theta_n\rangle_a$ .  $S$  and  $R$  matrix elements relate these states with others, where some of the rapidities have been switched, or had their sign changed. Using the known  $S$  and  $R$  matrices [9], correlators can then be computed [12], [22], provided one knows the matrix elements of the operators (form-factors) in the multiparticle basis [10]. For instance, for the energy density in the Ising model, the only non vanishing form-factors are

$$\langle \epsilon(w, \bar{w}) \rangle = \frac{m}{2} \int \frac{d\theta}{2\pi} R_a(\theta) \cosh \theta e^{-2imx \sinh \theta}, \quad (5)$$

and

$${}_a \langle 0 | \epsilon(w, \bar{w}) | \theta_1 \theta_2 \rangle_a = im e^{-my(\cosh \theta_1 + \cosh \theta_2)} \quad (6)$$

$$\times \prod_{k=1,2} [1 + R_b(\theta_k) t_k] \sinh\left(\frac{\theta_1 - \theta_2}{2}\right) e^{imx(\sinh \theta_1 + \sinh \theta_2)}$$

where  $t_i$  acts on functions of many variables by changing the sign of  $\theta_i$ , and  $R_b(\theta) = i \tanh\left(\frac{i\pi}{4} - \frac{\theta}{2}\right) \frac{\kappa_a - i \sinh \theta}{\kappa_a + i \sinh \theta}$ ,  $\kappa_a = 1 - \frac{h_a^2}{2m}$ .

The case where the theory is still massless in the bulk is the most interesting for applications [12]; it can simply be obtained as a massless limit of the previous description, with  $m \rightarrow 0$  and  $\theta \rightarrow \pm\infty$ .

Now suppose that the bulk mass is non zero, and in addition the boundary magnetic field is inhomogeneous:  $h = h_a$  for  $y \leq 0$  and  $h = h_b$  for  $y > 0$ . We now have two different hamiltonians to diagonalize, giving rise to two sorts of multiparticle eigenstates. Since these multiparticle eigenstates provide complete sets of states, the scalar products

$${}_b \langle \theta_n, \dots, \theta_1 | \theta_{n+1} \dots \theta_{n+m} \rangle_a \quad (7)$$

have to be non zero in general, even for disjoint sets of rapidities: they are nothing but the matrix elements of “boundary interactions changing operators”.

Knowledge of the scalar products (7) is what is required to compute a quantity like  $P(t)$ , as we will demonstrate later. For the moment, let us discuss how to determine these scalar products. Consider the simplest case,

$$\frac{{}_b \langle \theta_2 \theta_1 | 0 \rangle_a}{{}_b \langle 0 | 0 \rangle_a} = G(\theta_1, \theta_2). \quad (8)$$

Since for the Ising model, the integrable particles are just fermions with  $S = -1$ ,  $G$  must satisfy the exchange relations

$$G(\theta_1, \theta_2) = -G(\theta_2, \theta_1) = R_b^*(\theta_1) G(-\theta_1, \theta_2) \\ = R_b^*(\theta_2) G(\theta_1, -\theta_2). \quad (9)$$

In addition,  $G$  must have a kinematical pole at  $\theta_2 = \theta_1 - i\pi$ . To see this, observe that there are two possible expressions for the one point function of the energy: for  $y > 0$  one has

$$\langle \epsilon(w, \bar{w}) \rangle_{ba} = \int_0^\infty \frac{d\theta_1 d\theta_2}{8\pi^2} \{ {}_b \langle 0 | \epsilon(w, \bar{w}) | \theta_1 \theta_2 \rangle_b {}_b \langle \theta_2 \theta_1 | 0 \rangle_a \\ + {}_b \langle 0 | \epsilon(w, \bar{w}) | 0 \rangle_b {}_b \langle 0 | 0 \rangle_a \} / {}_b \langle 0 | 0 \rangle_a, \quad (10)$$

while for  $y < 0$ , one has

$$\langle \epsilon(w, \bar{w}) \rangle_{ba} = \int_0^\infty \frac{d\theta_1 d\theta_2}{8\pi^2} \{ {}_b \langle 0 | \theta_1 \theta_2 \rangle_a {}_a \langle \theta_2 \theta_1 | \epsilon(w, \bar{w}) | 0 \rangle_a \\ + {}_b \langle 0 | 0 \rangle_a {}_a \langle 0 | \epsilon(w, \bar{w}) | 0 \rangle_a \} / {}_b \langle 0 | 0 \rangle_a. \quad (11)$$

Replace now the form factors of  $\epsilon$  by their explicit forms: for (11) to be the analytical continuation of (10), we need the residue condition

$$\text{Res } G(\theta, \theta - i\pi) = -i \left( 1 - \frac{R_a(\theta)}{R_b(\theta)} \right) \quad (12)$$

This is enough to determine the function  $G$ . We find, using the parametrization  $\kappa_{a/b} = -\cosh \theta_{a/b}$ ,

$$G(\theta_1, \theta_2) = \frac{i}{8} \prod_{i=1,2} f(\theta_i) \frac{\sinh \theta_i}{\kappa_b + i \sinh \theta_i} \frac{\kappa_b + i \sinh \theta_i}{\kappa_b - i \sinh \theta_i} \times \frac{1}{\cosh(\frac{\theta_i}{2} + i\frac{\pi}{4})} \tanh\left(\frac{\theta_1 - \theta_2}{2}\right) \tanh\left(\frac{\theta_1 + \theta_2}{2}\right), \quad (13)$$

where

$$f(\theta) = \sqrt{-i(\kappa_a - \kappa_b)} \Phi(\theta|\theta_b, \theta_a) \Phi(\theta|-\theta_b, -\theta_a) \quad (14)$$

and

$$\Phi(\theta|\theta_b, \theta_a) \equiv \frac{1}{\cosh(\frac{\theta - \theta_b}{2} - i\frac{\pi}{4})} \prod_{n=0}^{\infty} \frac{\Gamma(\frac{5}{4} + n - i\frac{\theta - \theta_b}{2\pi})}{\Gamma(\frac{3}{4} + n - i\frac{\theta - \theta_b}{2\pi})} \frac{\Gamma(\frac{5}{4} + n + i\frac{\theta - \theta_b}{2\pi})}{\Gamma(\frac{3}{4} + n + i\frac{\theta - \theta_b}{2\pi})} \frac{\Gamma(\frac{3}{4} + n - i\frac{\theta - \theta_a}{2\pi})}{\Gamma(\frac{5}{4} + n - i\frac{\theta - \theta_a}{2\pi})} \frac{\Gamma(\frac{3}{4} + n + i\frac{\theta - \theta_a}{2\pi})}{\Gamma(\frac{5}{4} + n + i\frac{\theta - \theta_a}{2\pi})}. \quad (15)$$

Inspection shows that  $G$  has the same poles as those of  $R_b^*$ . Crossing in this problem reads  ${}_b\langle 0|\theta_1, \theta_2\rangle_a = {}_b\langle \theta_1 - i\pi, \theta_2 - i\pi|0\rangle_a$ . There is also a non trivial monodromy:  $G(\theta_1 + 2i\pi, \theta_2) = -R_a(\theta_1)R_b^*(\theta_1)G(\theta_1, \theta_2)$ .

Some comments are in order: the general solution for an arbitrary number of particles is not difficult to find and will be given in [23]. The previous expression depend only on  $h_{a/b}^2$ , and in fact, are only valid for  $h_a h_b > 0$ . The case of fields with opposite signs requires an additional particle at imaginary rapidity, see [23].

It is interesting now to get back to the conformal case: let  $m \rightarrow 0$  and, for instance,  $h_a = \infty$  and  $h_b = 0$ . Setting  $e = \pm p = e^\beta$ , we find from the foregoing formulas

$$\frac{+\langle \beta_2 \beta_1 | 0 \rangle_F}{+\langle 0 | 0 \rangle_F} = i \tanh \frac{\beta_1 - \beta_2}{2}, \quad (16)$$

where  $+$  designates up spins,  $F$  free spins. This is nothing but the form-factor of the  $\Delta = \frac{1}{16}$  operator, in agreement with [21]. We are then led to the following spectral representation for the energy one point function

$$\langle \epsilon(w, \bar{w}) \rangle_{+F} = -\frac{1}{4\pi x} + i \int \frac{d\beta_1 d\beta_2}{4\pi^2} e^{(\beta_1 + \beta_2)/2} \tanh\left(\frac{\beta_{12}}{2}\right) e^{ix(e^{\beta_1} - e^{\beta_2})} e^{-y(e^{\beta_1} + e^{\beta_2})}. \quad (17)$$

Explicit evaluation gives

$$\langle \epsilon(w, \bar{w}) \rangle_{+F} = \frac{1}{4\pi} \left( \frac{1}{x} - \frac{y}{x\sqrt{x^2 + y^2}} \right) - \frac{1}{4\pi x} \quad (18)$$

in agreement with the result obtained in [24] in the context of conformal field theory.

The scalar products (7) can be determined using the same ideas for more general integrable interacting theories. The expressions become quite bulky and won't be reproduced here; some very simple features determine most of  $P(t)$  properties, as we now explain.

The double well problem can be mapped on a single channel Kondo model when the dissipation is of ohmic type [14]. The hamiltonian reads

$$H_\lambda = \int_{-\infty}^0 dx \frac{1}{2} [\Pi^2 + (\partial_x \phi)^2] + \lambda \delta(x) (S_+ e^{i\sqrt{2\pi}g\phi} + S_- e^{-i\sqrt{2\pi}g\phi}). \quad (19)$$

The spins  $S_\pm$  are spin 1/2 operators, and the  $S_z$  value corresponds to the two states of the dissipative model. The dimensionless number  $g$  characterizes the dissipation. The quantity  $P(t)$  was defined in the introduction; it reads

$$P(t) = \langle 0 | S_z(t) | 0 \rangle \quad (20)$$

where  $|0\rangle$  is the product  $|0\rangle_{\lambda=0} \otimes |+\rangle$ ,  $|0\rangle_{\lambda=0}$  the ground state of the theory with  $\lambda = 0$ . The Heisenberg operator  $S_z(t)$  in (20) evolves with  $H_\lambda$ . To compute  $P(t)$ , we insert a complete set of eigenstates of  $H_\lambda$  on each side of  $S_z$ . These are multiparticle states resulting from the massless limit of the sine-Gordon model [3]; the spectrum is richer than in the Ising case and consists of solitons/anti-solitons, and, for  $g < 1/2$ , of breathers which we denote by  $\epsilon = \pm 1, 2, \dots$  respectively. The determination of  $P(t)$  then requires the scalar products  $\epsilon_p, \dots, \epsilon_1 \langle \beta_p, \dots, \beta_1 | 0 \rangle$ , which are of the same nature as those discussed previously, together with the form factors of the spin operator in the massless limit.

A subtle point has to be emphasized here: the integrable picture is an infrared one, where the spin is screened; that is, it doesn't appear in the multiparticle description. As demonstrated in [12] its properties can nevertheless be computed by using correlators of the current operator  $\partial_x \phi$  as follows

$$S_z(t) - S_z(0) = \int_0^t dt' \partial_x \phi(x=0, t'). \quad (21)$$

That the spin is up in the initial state is then taken into account by giving a unit charge to the state  $|0\rangle$ ; the non vanishing scalar products are thus those for which  $\sum \epsilon_i = 1$ .

At  $g = 1/2$  the sine-Gordon model decouples into two massless Ising models with a boundary magnetic field  $h \propto \lambda$  and the previous considerations on the Ising model can be used. There are no bound states at that point and the reflection matrix for the solitons and anti-solitons is

$$R_{+-} = R_{-+} = i \frac{e^\beta - iT_b}{e^\beta + iT_b}, \quad R_{++} = R_{--} = 0. \quad (22)$$

$T_b$  is describing the boundary scale and is related to  $\lambda$ , the precise relation to be found in Eq. (5.7) of [26]. The current operator has a simple form factor at that point given by (we turn to real time here)

$$\lambda \langle 0 | \partial_x \phi | \beta_1, \beta_2 \rangle_{\lambda}^{\epsilon_1, \epsilon_2} \propto \delta_{\epsilon_1 + \epsilon_2} \epsilon_1 e^{(\beta_1 + \beta_2)/2} \quad (23)$$

$$[1 + R_{+-}(\beta_1) R_{+-}(\beta_2)] e^{-it(e^{\beta_1} + e^{\beta_2})}. \quad (24)$$

We won't need the detailed knowledge of the scalar products (7); only their properties under crossing, together

with the value of the residues at the kinematical poles, matter.

Many processes contribute to the evaluation of  $P(t)$ . The simplest takes the form

$$\int \frac{d\beta_1 d\beta_2}{(2\pi)^2} {}_0\langle 0|\beta_2\rangle_{\lambda}^{++} \langle \beta_1|0\rangle_0 {}^+_{\lambda} \langle \beta_2|\partial_x \phi(t)|\beta_1\rangle_{\lambda}^+. \quad (25)$$

This process gets convoluted with many others, that is one has to add to the factor  $\langle 0|\beta_2\rangle_{\lambda}^{++} \langle \beta_1|0\rangle_0$  the sum

$$\int \frac{d\beta_3 d\beta_4}{(2\pi)^2} \langle 0|\beta_4\beta_3\beta_2\rangle_{\lambda}^{+-+} {}^{+-+}_{\lambda} \langle \beta_4\beta_3\beta_1|0\rangle + \dots \quad (26)$$

Suppose we move the rapidity integrals to  $\text{Im } \beta_1 = -i\pi$  and  $\text{Im } \beta_2 = i\pi$ . Forgetting the singularities encountered in doing so, one obtains, using crossing, the scalar product  ${}^+_{\lambda} \langle \beta_2|\beta_1\rangle_{\lambda}^+ = 2\pi\delta(\beta_1 - \beta_2)$ . But one easily checks that the form factor  ${}^+_{\lambda} \langle \beta|\partial_x \phi|\beta\rangle_{\lambda}^+$  vanishes, so the whole series adds up to zero! All what matters therefore are the contributions of the poles encountered in moving the contours. Moreover, one can show that the kinematical poles do not contribute; the one point function is entirely determined by the poles of the reflection matrix at  $\beta_{1,2} = \log(T_b) \mp i\pi/2$ . and one gets the well known result [14]

$$P(t) = e^{-2T_b t}. \quad (27)$$

The main feature of this computation - the fact that  $P(t)$  is entirely determined by the poles of the  $R$  matrices - generalizes to arbitrary values of  $g$ , since it follows entirely from the  $g$ -independent general properties of the scalar products. As a result, we can immediately obtain interesting properties. For  $g > 1/2$  there are only solitons and anti-solitons in the spectrum, for which the reflection matrix is independent of  $g$ , and still given by (22). It follows that the behaviour is entirely incoherent, and that  $P(t)$  has the form given in (1). All terms now contribute since the form factor of  $\partial_x \phi$  is non zero for any even number of particles at  $g > \frac{1}{2}$ .

When  $g < 1/2$  there are also  $m < [1/g]$  breathers in the spectrum ( $m$  integer), with a reflection matrix given by [25]

$$R_m(\theta) = -\frac{\tanh(\frac{\beta - \beta_b}{2} - i\frac{\pi m g}{4(1-g)})}{\tanh(\frac{\beta - \beta_b}{2} + i\frac{\pi m g}{4(1-g)})}, \quad (28)$$

with  $\beta_b = \log T_b$ . This matrix has poles where  $e^{\beta}$  has non vanishing real and imaginary part: they give rise to oscillatory contributions to  $P(t)$ , indicating that the behaviour is coherent in that domain. An expression similar to (1) can be written: the leading behaviour at large times (or small  $g$ ) follows from the one breather, as given in (2), leading to the ratio (3). This result is consistent with the expansion in  $g = 1/2 - \epsilon$  done in [17]. It also agrees with the  $g \rightarrow 0$  limit in which  $\lambda \approx \pi g T_b/2$

[26]. It would be very interesting to test this numerically. Formula (2) should be especially useful in the quantum optics context, where the values of  $g$  are usually quite small.

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